



To: Distribution List

From: Faculty Research Development Office (FRDO)
Office of the Vice President for Research

Subject: Limited Competition: DOE Computational Chemical Sciences (DE-FOA-0002426)

Date: November 10, 2020

UNM Researchers,

The Department of Energy (DOE) SC program in Basic Energy Sciences (BES) hereby announces its interest in receiving new and renewal applications from small groups (2-3 principal investigators) and integrated multidisciplinary teams (typically from multiple institutions) in Computational Chemical Sciences (CCS). Single-investigator applications are not responsive to the objectives of this FOA.

CCS will support basic research to develop validated, open-source codes for modeling and simulation of complex chemical processes and phenomena that allow full use of emerging exascale and future planned DOE leadership-class computing capabilities. The focus for CCS is on developing capabilities that allow modeling and simulation of new or previously inaccessible complex chemical systems and/or provide dramatic improvement in fidelity, scalability, and throughput. Teams should bring together expertise in domain areas (e.g., electronic structure, chemical dynamics, statistical mechanics, etc.) and other areas important to advance computational tools such as data science, algorithm development, and software architectures. **Priority will be given to efforts that address reaction chemistry across multiple scales in complex environments important in geosciences, catalysis, biochemistry, or electrochemistry.**

Applications that are responsive to this FOA will:

- Focus on development of open-source, community-based codes that can be deployed on emerging exascale and future leadership class computers to model systems of relevance to the BES mission, specifically those related to chemical sciences, geosciences, and biosciences.
- Focus on research leading to open-source software for description of chemical and molecular processes. Suitable types of software will address the intermediate to strong correlation and coupling regime, excited states, transport, dynamics, and/or electronic or optical properties, or will accurately describe the behavior of molecular quantum-information systems that are based upon high-fidelity processing of light, charge, or spin.
- Describe a plan to deliver validated research codes and the associated data to academia, National Laboratories, and industry. Software developed under this FOA should have broad applicability. All efforts should describe how their efforts will develop and deploy modular capabilities. Efforts must also describe their plan to distribute the software and foster community adoption.
- Provide a detailed plan for the full utilization of emerging exascale national leadership computing facilities.
- Explicitly excluded are proposals that are limited to use of existing quantum-based methods in their traditional regimes of application. Efforts aimed at extending currently attainable length/time

scales or increasing attention to complexity and that algorithmically match efficiency enhancements offered by next generation computers will receive priority.

Successful proposals will include strategies for realizing the full potential of exascale computers and for implementing algorithms that reduce the explicit complexity. Proposals will deploy methods that dramatically improve or go well-beyond those in use today.

Required pre-applications are due by **5pm EST on December 2nd** and encouraged applications are due February 8, 2021. Budgets will range from \$500,000 to \$2,000,000 per year for four years. More information can be found at <https://www.grants.gov/web/grants/view-opportunity.html?oppld=329588>.

This is a limited competition. Applicant institutions are limited to no more than two pre-applications and applications. Please follow the **required 2 steps** if you would like to participate on a proposal to the DOE.

Step 1 If you anticipate that you will be submitting a preproposal for this internal competition, please send a statement of interest naming the anticipated title of project, names and departments of all UNM personnel, and anticipated external collaborators (if applicable) via e-mail to limited@unm.edu by **noon, November 16, 2020**. Note: The statement of interest is required in order for the preliminary proposal to be reviewed by the limited competitions committee.

Step 2 Please submit your **2-page pre-proposal plus, rough budget overview, and short biosketches of members; all documents in a SINGLE PDF file, 11 point font by NOON on Friday, November 20, 2020 to limited@unm.edu with the subject line indicating: CCS - your name. No late submissions will be considered.**

The **pre-proposal narrative** must be in 11-point Times New Roman font with 1-inch margins and include:

- a) Title of Pre-application
Principal Investigator Name, Job Title
Institution
PI Phone Number, PI Email Address
FOA Number: Include the FOA Number indicated on the cover of this FOA
- b) This information must be followed by a clear and concise description of the objectives and technical approach of the proposed research.

Figures and references, if included, must fit within the two-page limit.